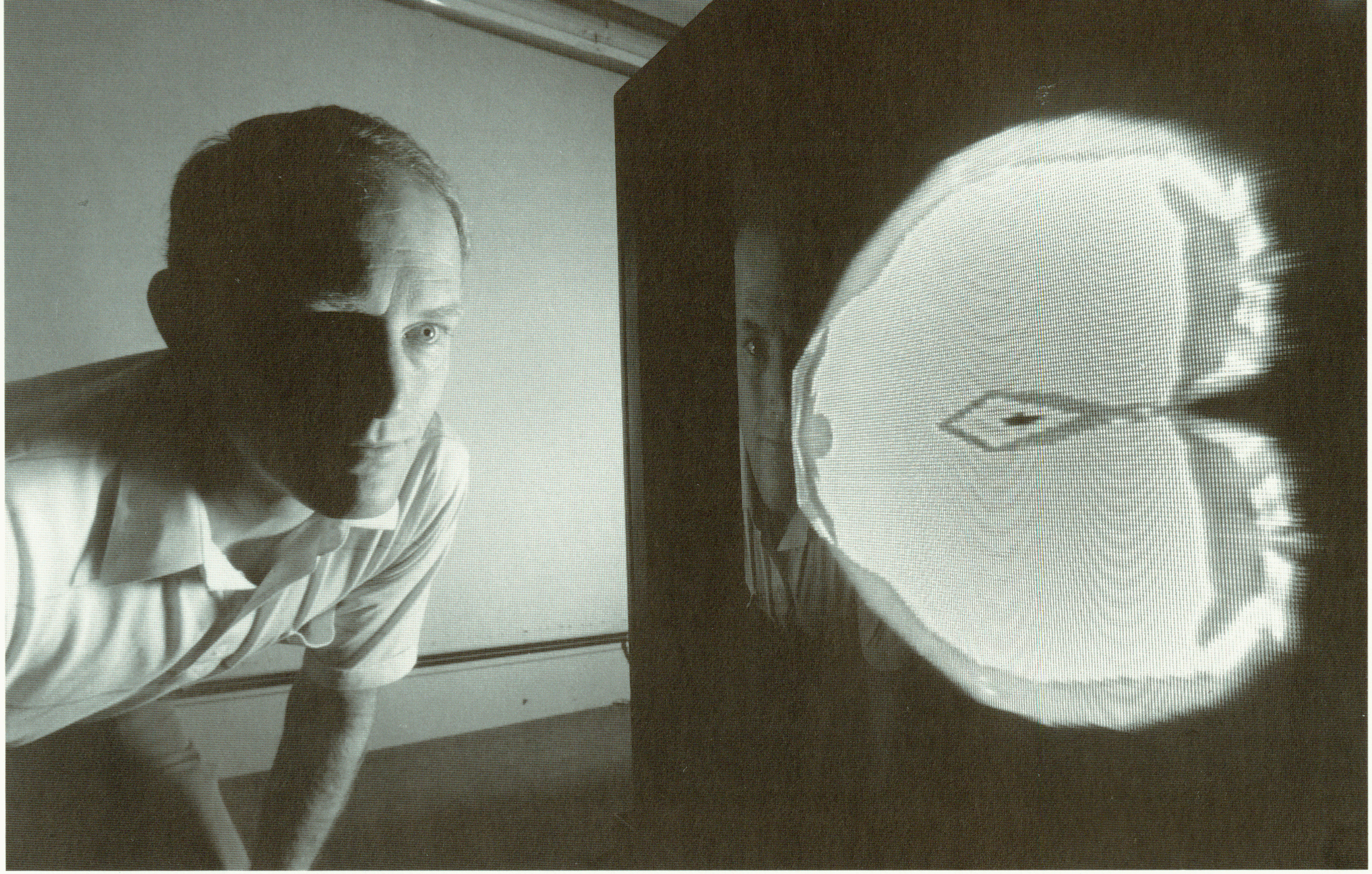

Chemist Gregory M. Glenn at the Western lab studies a 3-D computer model of a grain of wheat in research project to coax more flour from each kernel.

Computers for Research

It is safe to say that every scientist today uses computers in some way to carry out research. Typically, the Northern center has a central scientific data processor to serve needs of the whole laboratory. It is used to collect raw data, perform mathematical analyses, augment instruments, produce reports, and store the data. It is an indispensable research assistant.

On some projects, however, the computer is more than that. A scientist at the Southern center, for example, insists that the computer is his "primary research instrument." It enables him, he says, to predict the physical shape of large molecules, often with minimal experimental data.

It is not enough for a chemist to know the kinds and numbers of atoms in many organic molecules, such as starch or cellulose. The physical properties of compounds also depend on the shape and configuration of the molecules. It is often difficult, however, to determine three-dimensional structures of many giant molecules through laboratory experiments.

The SRRC modeling project has already resulted in the first precise description of the double-helix shape of a starch molecule, a structure now generally accepted by the scientific world. A current project seeks to determine the energies of different shapes of sugar rings, based on research conducted by an SRRC scientist in the pre-computer days of the 1940's. At that time, he worked out on paper all the possible shapes of sugar rings. Today's computer research is an outgrowth of those pioneering studies more than 40 years ago.

Comparable modeling with computers is taking place at the Northern center. Under study are long molecules of triglycerides, fatty acids, and lipids that contain large proportions of carbon and hydrogen. Some of these compounds are essential to life; others are harmful if ingested but essential for many home, automotive, and industrial uses. Unsaturated fats are good for dietary purposes, for instance; saturated fats, not so good.

Fat molecules are able to perform many different tasks because they contain long chains of carbon atoms that tend to associate with each other and form larger molecular aggregates, each with different properties. Because of their chemical structures, chains of carbon atoms in saturated fats tend to be straight, while those in unsaturated fats are bent. Fat molecules can also take on different shapes and dimensions that can change with ease, depending on the conditions under which the fat is used. This ability to assume many different forms makes fats useful, but it can complicate fitting the fat to the task. With modern computer software and knowledge of the specific properties that are required of a fat molecule, chemists can build molecules atom by atom, move them around, and change their shape. Finally, they can determine whether the molecule's shape and packing will provide the properties needed for a particular task. Soon chemists will be able to identify the best fat molecule for each purpose, whether for the human diet or for industry.

At the Western center, three-dimensional computer modeling is a powerful tool to help researchers improve their understanding of milling wheat. Wheat flour is made by stripping away the outer bran layer of wheat kernels and crushing the endosperm, the inner tissue that produces the flour. About 8 percent of the endosperm remains stuck to the bran and is lost during milling. If more of the endosperm could be separated from the bran, it would mean a tremendous increase in flour production. Just as a 3-D computer model can help pinpoint where an engine is most likely to fail, it can also predict how a kernel of wheat will respond to various preconditioning and crushing treatments. Western center scientists are confident that computer modeling will eventually enable millers to fine-tune their milling practices to achieve higher yields of flour.

The Eastern center has come up with a different sort of computer program. Faced with higher energy costs, more stringent environmental rules, and requirements for nutritional labeling, managers of food processing plants are more concerned than ever with increasing the efficiency of their operations. To help them do this, ERRC researchers have created a computer program and models applicable to many different types of industrial activity. Called the ERRC Food Process Simulator, it was designed to help processors achieve not only higher production and profits, but also a more nutritious product made in a more energy-efficient manner. The program can be used to make theoretical changes in a production process on a computer without the cost and disruption of actually making the physical alterations in the plant. It can be applied to parts of a process as well as to the whole production system. Since the ERRC program and models were developed, more than 100 organizations have obtained copies and are modeling industrial processes for such diverse commodities as potatoes, crackers, cheese, beer, corn, chocolate, and pharmaceuticals.

In another Eastern lab unit, scientists had for many years studied the proteins in casein (from milk) and collagen (from hides) to improve their function and utilization. While a great deal of physical chemistry data had been collected on these proteins, the exact molecular structure remained elusive until the computer came along. Today ERRC researchers construct theoretical 3-D models of these noncrystalline proteins in the computer, based on the amino acid sequence. They then adjust the models to incorporate known physico-chemical details. The computer simulation usually suggests further experiments to verify each model, and the new data are used to refine it even more. Molecular models help researchers to predict, among other things, the optimal conditions for processing the proteins into useful products. They also help scientists to understand how each protein functions in the animal's body.